201-15004

Elizabeth Hunt
<ehunt@adelphia.net>
12/30/03 02:40 PM

To: Rtk Chem@EPA, NCIC OPPT@EPA
cc: Leslie Scott/DC/USEPA/US@EPA, Richard Hefter/DC/USEPA/US@EPA
Subject: Ketones: Submission for 4-Heptanol, 2,6-dimethyl- (CAS 108-82-7) Under HPV Program

Attached is a submission on behalf of The Dow Chemical Company (as part of the Lesser Ketones Manufacturing Association commitment) for 4-Heptanol, 2,6-dimethyl- (CAS 108-82-7), under the US HPV Program.

This submission includes the following attached files:

- Test Plan
- IUCLID Dossier

If you have any difficulty opening these files or have any questions, please contact me.

Elizabeth Hunt

Executive Director


DIBC_108-82-7 Test Plan 121903 FINAL.doc


DIBC_108-82-7 IUCLID 21903 FINAL.rtf

201-15004

4-Heptanol, 2,6-dimethyl-

(Diisobutyl Carbinol; CAS RN 108-82-7)

High Production Volume (HPV) Chemical Challenge Test Plan and Data Review

Prepared for:

The Dow Chemical Company

Prepared by:

Toxicology/Regulatory Services, Inc.

December 19, 2003

4-Heptanol, 2,6-dimethyl-
(Diisobutyl Carbinol; CAS RN 108-82-7)
High Production Volume (HPV) Chemical Challenge
Test Plan and Data Review

Table of Contents Page

Tables

Test Plan

4-Heptanol, 2,6-dimethyl- **(Diisobutyl Carbinol; CAS RN: 108-82-7)**		Information	OECD Study	GLP	Other Study	Estimation Method	Acceptable	Testing Required
STUDY		**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**
PHYSICAL AND CHEMICAL DATA								
2.1	Melting Point	Y	N	N	Y	N	Y	N
2.2	Boiling Point	Y	N	N	Y	N	Y	N
2.4	Vapor Pressure	Y	N	N	Y	N	Y	N
2.5	Partition Coefficient	Y	N	N	N	Y	Y	N
2.6	Water Solubility	Y	N	Y	Y	N	Y	N
ENVIRONMENTAL FATE AND PATHWAY								
3.1.1	Photodegradation	Y	N	N	N	Y	Y	N
3.1.2	Stability in Water	Y	N	N	Y	N	Y	N
3.3	Transport and Distribution	Y	N	N	N	Y	Y	N
3.5	Biodegradation	Y	Y	Y	N	N	Y	N
ECOTOXICITY								
4.1	Acute Toxicity to Fish	Y	Y	Y	N	N	Y	N
4.2	Toxicity to Daphnia	Y	Y	Y	N	N	Y	N
4.3	Acute Toxicity to Algae	Y	Y	Y	N	N	Y	N
TOXICITY								
5.1	Acute Toxicity	Y	N	N	Y	N	Y	N
5.4	Repeated Dose Toxicity	N	N	N	N	N	N	**Y**
5.5	Genotoxicity *In Vitro* (Bacterial Test)	Y	Y	Y	N	N	Y	N
5.5	Genotoxicity *In Vitro* (Mammalian Cells)	N	N	N	N	N	N	**Y**
5.8	Reproductive Toxicity	N	N	N	N	N	N	**Y**
5.9	Development Toxicity / Teratogenicity	N	N	N	N	N	N	**Y**

4-Heptanol, 2,6-dimethyl-
(Diisobutyl Carbinol; CAS RN 108-82-7)
High Production Volume (HPV) Chemical Challenge
Test Plan and Data Review

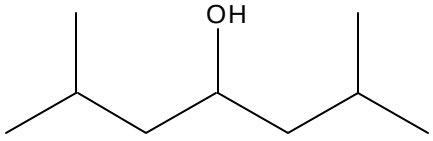
1.0 Introduction

This document provides a Test Plan and reviews the data availability for the High Production Volume (HPV) Chemical Challenge endpoints for 4-Heptanol, 2,6-Dimethyl-, hereafter called Diisobutyl Carbinol [DIBC; CAS RN 108-82-7]. DIBC is sponsored by The Dow Chemical Company.

2.0 General Use and Exposure

Diisobutyl Carbinol (DIBC) has a number of small volume uses. It is commonly used in mining, fabric softeners and textile and paper manufacturing. DIBC also is a lubricant additive intermediate, defoamer in adhesives, a coupling solvent for synthetic resins, a dispersing agent in coatings, and a chemical manufacturing processing solvent. Small amounts of DIBC are used in the fragrance industry as a chemical intermediate in the production of perfumes and/or flavors. Over 90% of the U.S. production of DIBC is as a chemical process solvent in the production of hydrogen peroxide. During 2002, 1 to 3 million pounds of DIBC were produced in the United States.

3.0 General Substance Information (Identity)

Chemical Name	4-Heptanol, 2,6-Dimethyl-
Synonyms	Diisobutyl Carbinol 2,6-Dimethyl heptanol-4 2,6-Dimethyl-4-heptanol 4-Heptanol, 2,6-dimethyl- 4-Hydroxy-2,6-dimethyl heptane Diisobutylcarbinol Nonyl alcohol, secondary sec-Nonyl alcohol
CAS Number	108-82-7
Structure	
Molecular Weight	144.26
Substance Type	Organic
Physical State	Liquid
Odor	Sweet
Purity	2,6-dimethyl-4-heptanol (DIBC) 70% 4,6-dimethyl-2-heptanol (DMH) 30% 2,6-dimethyl-4-heptanone 3%

4.0 Physical/Chemical Properties

A data summary for DIBC is included in Table 1. The Robust Summaries are included in the IUCLID Dataset.

4.1 Melting Point

The melting point for DIBC is listed as –65.2 °C (DIPPR, 2000). This value is considered adequate to meet the HPV Chemical Challenge requirements.

4.2 Boiling Point

The boiling point for DIBC is listed as 177.9 °C (DIPPR, 2000). This value is considered adequate to meet the HPV Chemical Challenge requirements.

4.3 Vapor Pressure

The vapor pressure for DIBC is listed as 0.260 hPa at 20 °C (DIPPR, 2000). This value is considered adequate to meet the HPV Chemical Challenge requirements.

4.4 Partition Coefficient

The log K_{ow} for DIBC is predicted by EPIWIN to be 3.08 (U.S. EPA, 2000a). This value is consistent with the known properties of DIBC and is considered adequate to meet the HPV Chemical Challenge requirements.

4.5 Water Solubility

The water solubility value for DIBC was determined to be 570 mg/L (Wilson, 2000). This value is considered adequate to meet the HPV Chemical Challenge requirements.

5.0 Environmental Fate

A data summary for DIBC is included in Table 1. The Robust Summaries are included in the IUCLID Dataset.

5.1 Photodegradation

The model prediction for atmospheric photodegradation provides a second order rate of reaction with hydroxyl radicals of 18.7 E-12 cm^3/molecule-sec and a $t_{1/2}$ of 6.9 hours (U.S. EPA, 2000b). Because of the nature of use of DIBC, photodegradation is of minimal importance to the overall environmental fate. Rapid degradation from accidental release to the atmosphere, however, is anticipated based on the modeling. These data are considered adequate to meet the HPV Chemical Challenge requirements.

5.2 Stability in Water

DIBC does not react with water; the only functionality other than carbon-carbon and carbon-hydrogen bonds is the hydroxyl group, which does not hydrolyze.

5.3 Transport and Distribution

The Level III fugacity model (U.S. EPA, 2000c) was used to predict the distribution of DIBC released into the environment. Environmental exposure to DIBC is limited based on the use patterns as an industrial intermediate and solvent. For example, DIBC is not listed on the Toxic Release Inventory. Therefore, only accidental releases were considered for the fugacity modeling. Two scenarios, 100% release to air and 100% release to water were examined. For the air release, the model predicted a distribution of 90% into atmosphere, 8% into water, 2% into soil, and < 1% into sediment. For the water release, the model predicted a distribution of 1% into atmosphere, 97% into water, < 0.1% into soil, and 1% into sediment. These data are considered adequate to meet the HPV Chemical Challenge requirements.

5.4 Biodegradability

A study measuring the biodegradation of DIBC in an OECD 301F respirometer test under aerobic conditions for 28 days found that the DOC removal was 99.5% by Day 28; the ThOD reached 10% by Day 8 and 53% in the next 10 days, attaining 60% by Day 28. The author concluded that DIBC is not readily biodegradable because the strict criterion for the 10-day window was not met (Heim, 2003). DIBC can be classified as inherently biodegradable and nearly meets the criteria for ready biodegradation in this test system. These data are considered adequate to meet the HPV Chemical Challenge requirements.

6.0 Ecotoxicity

A data summary for DIBC is included in Table 1. The Robust Summaries are included in the IUCLID Dataset.

6.1 Toxicity to Fish

The 72- and 96-hour LC_{50} value for DIBC toxicity to freshwater fish (rainbow trout; *Oncorhynchus mykiss*) is reported as 28.6 mg/L (Marino and Yaroch, 2002a). The study was conducted in compliance with EPA OTS Guideline 797.1400 except that DIBC concentrations were not measured in the test solutions and nominal values were used throughout. Because DIBC does not hydrolyze, the nominal concentrations are acceptable and this LC_{50} value is considered adequate to meet the HPV Chemical Challenge requirements.

6.2 Toxicity to Aquatic Invertebrates

The 48-hour EC_{50} value for DIBC toxicity to *Daphnia magna* is 47.8 mg/L (Marino and Yaroch, 2002b). The study was conducted in compliance with EPA OTS Guideline 797.1300 except that DIBC concentrations were not measured in the test solutions and nominal values were used throughout. Because DIBC does not hydrolyze, the nominal concentrations are acceptable and this EC_{50} value is considered adequate to meet the HPV Chemical Challenge requirements.

6.3 Toxicity to Aquatic Plants

The 96-hour EC_{50} values for DIBC toxicity based on biomass and growth rate to *Selenastrum capricornutum* (algae) are 7.41 and 29.95 mg/L, respectively (Roshon, 2002). The study was conducted in compliance with OECD Guideline 201. These data are considered adequate to meet the HPV Chemical Challenge requirements.

7.0 Human Health-Related Data

A data summary for DIBC is included in Table 1. The Robust Summaries are included in the IUCLID Dataset.

7.1 Acute Toxicity

The following acute toxicity data are available: acute oral LD_{50} in rats = 3560 mg/kg bw; acute dermal LD_{50} in rabbits = 4591 mg/kg bw; no deaths from an 8-hr exposure to substantially saturated vapor or cooled mist of DIBC (Carpenter, 1948). These data are considered adequate to meet the HPV Chemical Challenge requirements.

7.2 Repeated Dose Toxicity

No data were identified for repeated dose toxicity. An oral (gavage) study using OECD Guideline 422 is in progress.

7.3 Genetic Toxicity (*in vitro*)

DIBC has been shown to be negative in a high quality Bacterial Reverse Mutation assay for *Salmonella* and *E. coli* strains with and without metabolic activation (Mecchi, 2002). A study to evaluate chromosomal aberrations using OECD Guideline 473 is in progress.

7.4 Reproductive and Developmental Toxicity

No data were identified for reproductive or developmental toxicity. An oral (gavage) study using OECD Guideline 422 is in progress.

8.0 Conclusion

Adequate information is available for melting point, boiling point, vapor pressure, partition coefficient and water solubility for DIBC. Photodegradation and environmental distributions are adequately supported by the appropriate model data. DIBC does not have hydrolyzable groups and is stable in abiotic aqueous systems and is biodegradable. Aquatic toxicity data are available for fish, daphnia and algae indicating that DIBC is moderately toxic to aquatic organisms. DIBC is relatively non-toxic via acute oral, dermal and inhalation exposure. In bacterial cell systems, DIBC is not mutagenic. Additional testing is in progress for repeated dose, reproductive and developmental screening using the OECD 422 protocol. In addition, a chromosomal aberration assay (OECD 473) is in progress. The available data and the studies in progress are considered adequate to meet the HPV Challenge Program requirements.

9.0 References

Carpenter, C.P. 1948. Range Finding Tests on Diisobutyl Carbinol. Unpublished Report Number 11-89. Mellon Institute of Industrial Research, University of Pittsburgh, PA, USA.

DIPPR (The Design Institute for Physical Properties). 2000. The DIPPR Information and Data Evaluation Manager, Version 1.5.0, Copyright BYU-TPL2000.

Heim, D. 2003. Diisobutyl carbinol: Determination of Ready Biodegradability Using the Respirometry Method. Unpublished Report (ABC No. 47679; Dow No. 020112) for The Dow Chemical Company by ABC Laboratories, Inc., Columbia, MO, USA.

Marino, T. A. and A. M. Yaroch. 2002a. Diisobutyl Carbinol: An Acute Toxicity Study with the Rainbow Trout, *Oncorhynchus mykiss* Walbaum. Unpublished Report (Dow No. 021047) for Union Carbide Corporation by Toxicology & Environmental Research and Consulting, The Dow Chemical Company, Midland, MI, USA.

Marino, T. A. and A. M. Yaroch. 2002b. Diisobutyl Carbinol: An Acute Toxicity Study with the Daphnid, *Daphnia magna* Straus. Unpublished Report (Dow No. 021048) for Union Carbide Corporation by Toxicology & Environmental Research and Consulting, The Dow Chemical Company, Midland, MI, USA.

Mecchi, M. S. 2002. *Salmonella – Escherichia coli*/Mammalian-Microsome Reverse Mutation Assay Preincubation Method with a Confirmatory Assay with Diisobutyl Carbinol. Unpublished Report (Covance Study No. 23500-0-422OECD; Dow No. 011222) for The Dow Chemical Company by Covance Laboratories Inc., Vienna, VA, USA.

Roshon, R. 2002. Diisobutyl Carbinol: Growth Inhibition Test with the Freshwater Green Alga, *Selenastrum capricornutum* Printz. Unpublished Report (ESG Study No. S2287; Dow No. 020026) for the Dow Chemical Company by ESG International Inc., Guelph, Onterio, Canada.

U.S. EPA (U.S. Environmental Protection Agency). 2000a. EPI Suite™, Version 3.10; KOWWIN Program, Version 1.66; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

U.S. EPA (U.S. Environmental Protection Agency). 2000b. EPI Suite™, Version 3.10; AOPWIN Program, Version 1.90; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

U.S. EPA (U.S. Environmental Protection Agency). 2000c. EPI Suite™, Version 3.10; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Wilson, L. C. 2000. Liquid-Liquid Equilibrium Measurements for Eighteen Glycol Ethers, Ketones, Esters and Alcohols with Water. Project Report No. 44662, 10/13/2000. Union Carbide Corporation, S. Charleston, WV, USA.

Table 1: HPV Data Summary

4-Heptanol, 2,6-Dimethyl-
(Diisobutyl Carbinol; DIBC)

CAS RN: 108-82-7		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point		Handbook Data (DIPPR)	-65.2 °C
2.2	Boiling Point		Handbook Data (DIPPR)	177.9°C
2.3	Density		Handbook Data (DIPPR)	0.8112 g/cm^3 (at 20 °C)
2.4	Vapor Pressure		Handbook Data (DIPPR)	0.260 hPa (at 20 °C)
2.5	Partition Coefficient (log K_{ow})		KOWWIN v 1.66	3.08
2.6	Water Solubility		ASTM E 1148	570 mg/L (at 20 °C)
2.7	Flash Point		Handbook Data (DIPPR)	65.85 ºC
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		AOPWIN v. 1.90	half-life: 6.9 hours (OH Rate Constant)
3.1.2	Stability in Water		Hydrolysis @ 25 °C	Does not react with water; the only functionality other than carbon-carbon and carbon-hydrogen bonds is the hydroxyl group which does not hydrolyze
3.3	Transport and Distribution		Mackay Level III 100% release to air;	90% into atmosphere, 8% into water, 2% into soil, < 1% into sediment
			Mackay Level III 100% release to water	1% into atmosphere, 97% into water, < 0.1% into soil, 1% into sediment
3.5	Biodegradation		OECD 301F	ThOD = 60% after 28 days
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	*Oncorhynchus mykiss*	OTS 797.1400	LC_{50} (96 hours) = 28.6 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates	*Daphnia magna*	OTS 797.1300	EC_{50} (48 hours) = 47.8 mg/L
4.3	Toxicity to Aquatic Plants e.g. Algae	*Selenastrum capricornutum*	OECD Guideline 201	EC_{50} (96 hours) 7.41 mg/L (biomass) 29.95 mg/L (growth rate)

Table 1: HPV Data Summary

4-Heptanol, 2,6-Dimethyl-
(Diisobutyl Carbinol; DIBC)

CAS RN: 108-82-7		SPECIES	PROTOCOL	RESULTS
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat		LD50 : 3560 mg/kg bw
5.1.2	Acute Inhalation Toxicity	Rat		No deaths following 8-hr exposure to saturated vapor or cooled mist
5.1.3	Acute Dermal Toxicity	Rabbit		LD_{50}: 4591 mg/kg bw
5.4	Repeated Dose Toxicity	Rat	OECD 422	Study in progress
5.5	Genetic Toxicity *In Vitro*			
	Bacterial Test (Gene mutation)	*S. typhimurium and E. coli*	OECD 471	Negative
	Chromosomal Aberration	CHO	OECD 473	Study in progress
5.8	Toxicity to Reproduction / Impairment of Fertility	Rat	OECD 422	Study in progress
5.9	Developmental Toxicity / Teratogenicity	Rat	OECD 422	Study in progress

201-15004

I U C L I D

Data Set

Existing Chemical	:	ID: 108-82-7
CAS No.	:	108-82-7
EINECS Name	:	2,6-dimethylheptan-4-ol
EC No.	:	203-619-6
TSCA Name	:	4-Heptanol, 2,6-dimethyl-
Molecular Formula	:	C9H20O
Producer related part		
Company	:	The Dow Chemical Company
Creation date	:	12.09.2003
Substance related part		
Company	:	The Dow Chemical Company
Creation date	:	12.09.2003
Status	:	
Memo	:	
Printing date	:	18.12.2003
Revision date	:	
Date of last update	:	18.12.2003
Number of pages	:	26
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name	:	
Smiles Code	:	OC(CC(C)C)CC(C)C
Molecular formula	:	C9 H20 O1
Molecular weight	:	144.26
Petrol class	:	

05.12.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	typical for marketed substance
Substance type	:	organic
Physical status	:	liquid
Purity	:	-
Colour	:	Transparent colorless
Odour	:	Sweet
Remark	:	Purity/composition: >=70% 2,6-diemthyl-4-hepatanol (DIBC) <=30% 4,6-dimethyl-2-hepatnol (DMH) <=3% 2,6-dimethyl-4-heptanone

05.12.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2,6-Dimethyl heptanol-4

04.12.2003

2,6-Dimethyl-4-heptanol

04.12.2003

4-Heptanol, 2,6-dimethyl-

04.12.2003

4-Hydroxy-2,6-dimethyl heptane

04.12.2003

Diisobutyl Carbinol

04.12.2003

Diisobutylcarbinol

04.12.2003

Nonyl alcohol, secondary

04.12.2003

sec-Nonyl alcohol

04.12.2003

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : = -65.2 - °C

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
04.12.2003 (7)

2.2 BOILING POINT

Value : = 177.9 - °C at 1013 hPa

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
04.12.2003 (7)

2.3 DENSITY

Type : density
Value : = .8112 - g/cm³ at 20 °C

08.10.2003 (7)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .25955 - hPa at 20 °C

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
04.12.2003 (7)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 3.08 - at °C
pH value : -
Method : other (calculated): EPIWIN (v 3.10) KOWWIN Submodel (v 1.66)
Year : 2003
GLP :
Test substance :

Remark : The EPIWIN model was run using the following measured physical chemical properties:
Vapor pressure (mm Hg) = 0.19515;
Boiling point (deg C) = 177.85; and
Melting point (deg C) = -65.15.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
04.12.2003 (10)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 570 - mg/l at 20 °C
pH value	:	-
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Broadly covered by ASTM method E 1148
Year	:	2000
GLP	:	yes
Test substance	:	other TS

Remark : The liquid-liquid equilibrium measurements were performed in a 2.0 liter glass vessel submerged in a constant-temperature bath. Water and DIBC were added to this vessel through 1/16" lines. The mixture was then stirred vigorously by a magnetic stirrer at the desired bath temperature. Stirring produced very fine droplets of each phase entrained in the other phase, which slowly separated after the liquid was still. After the liquid phases had separated, three 20-30 gram samples were withdrawn from the aqueous liquid phase into weighed glass bottles. A weighed amount of a mixture of toluene and dodecane was added to each vial of the aqueous phase, and the DIBC was extracted into the toluene-rich phase by vigorously shaking the vial. Dodecane served as the internal standard. An aliquot of the toluene-rich phase was then analyzed by gas chromatography. The concentration of water was found by difference. The gas chromatographic analyses were performed by an HP5890 II gas chromatograph equipped with a DB-1 capillary column. The column was 30 meters long with an internal diameter of 0.32 millimeters and a film thickness of 3 micrometers. Response factors were determined by analyzing gravimetrically prepared standards before each set of samples.

Three 5-10 gram samples of the hydrocarbon phase were withdrawn into weighed syringes. The contents of each syringe were flushed into the Karl-Fisher titrator by first injecting as much liquid as possible from the syringe into the titrator vessel. Then a long needle was used to pull the titrant and solvent from the titration vessel into the syringe, shaking the syringe to mix the it, and then injecting the liquid back into the titration vessel. The sample was then titrated. The titrant was calibrated by titrating weighed aliquots of distilled water.

Result : In all samples there was excellent separation of the phases. Results were repeated in triplicate. Compositions between one weight percent and 0.1 wt% are estimated to be reliable to ±5% of the reported value. The uncertainty increases to ±20% of the reported value as the measured compositions decrease to the ppm level.

Test substance : 2,6-dimethyl-4-heptanol, DIBC
Purity > 96 wt%

Reliability : (1) valid without restriction
Comparable to guideline study.

Flag : Critical study for SIDS endpoint

05.12.2003 (12)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 65.9 °C
Type :

02.10.2003 (7)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	other: EPIWIN (v 3.10) AOPWIN Submodel (v 1.90)
Light source	:	
Light spectrum	:	- nm
Relative intensity	:	- based on intensity of sunlight
DIRECT PHOTOLYSIS		
Halflife t1/2	:	= 6.9 - hour(s)
Degradation	:	- % after
Quantum yield	:	
Deg. product	:	
Method	:	other (calculated): EPIWIN (v 3.10) AOPWIN Submodel (v 1.90)
Year	:	2003
GLP	:	
Test substance	:	
Remark	:	Overall OH rate constant = 18.6802 E-12 cm3/molecule/sec The EPIWIN model was run using the following measured physical chemical properties: Vapor pressure (mm Hg) = 0.19515; Boiling point (deg C) = 177.85; and Melting point (deg C) = -65.15.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

05.12.2003 (8)

3.1.2 STABILITY IN WATER

Remark	:	Expert Statement: DIBC does not react with water; the only functionality other than carbon-carbon and carbon-hydrogen bonds is the hydroxyl group which does not hydrolyze.

04.12.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media	:	other: air (emissions to compartment = 1000 kg/hr)
Method	:	Calculation according Mackay, Level III
Year	:	2003
Remark	:	The EPIWIN model was run using the following measured physical chemical properties:

Vapor pressure (mm Hg) = 0.19515;
Boiling point (deg C) = 177.85; and
Melting point (deg C) = -65.15.

Result : Concentration (%):
Air = 90
Water = 8
Soil = 2
Sediment = <1

Level III Fugacity Model (Full-Output):
==========
Chem Name : 4-Heptanol, 2,6-dimethyl-
Molecular Wt: 144.26
Henry's LC : 0.000129 atm-m3/mole (Henry database)
Vapor Press : 0.195 mm Hg (user-entered)
Log Kow : 3.08 (Kowwin program)
Soil Koc : 493 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	90.4	13.7	1000
Water	7.85	360	0
Soil	1.67	360	0
Sediment	0.0955	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.79e-011	831	165	83.1	16.5
Water	6.39e-012	2.75	1.43	0.275	0.143
Soil	1.24e-012	0.585	0	0.0585	0
Sediment	3.03e-012	0.00837	0.000348	0.000837	3.48e-005

Persistence Time: 18.2 hr
Reaction Time: 21.9 hr
Advection Time: 110 hr
Percent Reacted: 83.4
Percent Advected: 16.6

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 13.74
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 3.040 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
07.12.2003 (11)

Media : other: water (emissions to compartment = 1000 kg/hr)
Method : Calculation according Mackay, Level III
Year : 2003

Remark : The EPIWIN model was run using the following measured physical chemical properties:
Vapor pressure (mm Hg) = 0.19515;
Boiling point (deg C) = 177.85; and
Melting point (deg C) = -65.15.

Result : Concentration (%)
Air = 1
Water = 97
Soil < 0.1
Sediment = 1

Level III Fugacity Model (Full-Output):
==========
Chem Name : 4-Heptanol, 2,6-dimethyl-
Molecular Wt: 144.26
Henry's LC : 0.000129 atm-m3/mole (Henry database)
Vapor Press : 0.195 mm Hg (user-entered)
Log Kow : 3.08 (Kowwin program)
Soil Koc : 493 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.38	13.7	0
Water	97.4	360	1000
Soil	0.0255	360	0
Sediment	1.18	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	6.35e-012	189	37.5	18.9	3.75
Water	1.18e-009	508	264	50.8	26.4
Soil	2.83e-013	0.133	0	0.0133	0
Sediment	5.59e-010	1.54	0.0642	0.154	0.00642

Persistence Time: 271 hr
Reaction Time: 388 hr
Advection Time: 899 hr
Percent Reacted: 69.9
Percent Advected: 30.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 13.74
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 3.040 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
07.12.2003 (11)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : other
Concentration : 33.4 mg/l related to
related to

Contact time	:	28 day(s)
Degradation	:	- 60 (±) % after 28 day(s)
Result	:	other
Kinetic of testsubst.	:	8 day(s) > - 10 % 18 day(s) - 18 % 28 day(s) - 60 % - % - %
Control substance	:	Benzoic acid, sodium salt
Kinetic	:	28 day(s) > - 90 % - %
Deg. product	:	not measured
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	2003
GLP	:	yes
Test substance	:	other TS
Method	:	This study investigated the biodegradation of the test substance in respirometers under aerobic conditions for 28 days. Duplicate 500-ml test solutions were prepared by adding mineral salts medium, reagent water, the activated sludge inoculum (6.0x106 CFU/ml) and test substance (added by weight) to 1-L flasks to achieve a nominal ThOD of 100 mg/l. Negative controls, abiotic controls (100 mgThOD/l) and reference controls (sodium benzoate, 60 mg/L or 100 mgThOD/l) were similarly prepared, only the negative control in duplicate, and concurrently maintained. The flasks were continuously stirred during incubation in water bath at 22±2°C in the dark. Oxygen in the sealed headspace above each solution was measured every 6 hours. The pH and DOC concentration were measured in each flask at test termination. Bacterial plate counts were performed for the prepared activated sludge and a sample of each test solution collected on Day 28. Due to the high DOC removal from the abiotic control, the test was repeated after changing selected parameters in an effort to reduce possible volatilization and improve the efficiency of the respirometer. The values reported herein reflect the results of the second test.
Remark	:	Activated sludge suspension was collected from aeration basin #1 of the Columbia Wastewater Treatment Plant, Columbia, Missouri.
Result	:	The pH in all of the flasks ranged from 7.23 to 7.39, and averaged 7.37 and 7.23 in the test substance replicates at initiation and termination, respectively. The bacterial plate counts at termination showed that the test substance solutions contained an average of 1.12x105 CFU/ml. Degradation based on DOC removal reached 99.5% by Day 28. The percent ThOD exceeded 10% ThOD by Day 8 in both replicates and further degraded to an average 53% ThOD by Day 18 (the end of the 10-day window). By test termination, ThOD reached 60%, thus this test substance is considered to be not readily biodegradable under the conditions of this test in spite of the rapid biodegradation phase between days 7 and 11 and almost complete removal of DOC. Since volatilization was minimized during this test, the additional 40% difference in biodegradation seen as DOC removal was attributed to adsorption. This conclusion was supported by the 56% degradation as DOC removal observed for the sterile control (versus the 7.2% ThOD). The percent ThOD for the reference substance was >90% by Day 28, proving that the inoculum was viable.
Test substance	:	See Section 1.1; Purity: DIBC + DMH = 99.4%; The purity of the test substance was not included in the report but the Lot Number used was the same as for the Acute Fish Toxicity and Acute Invertebrate Toxicity studies for which the purity was determined.
Conclusion	:	Not readily biodegradable under the conditions of thi s test, as '10-day window' was not met (Author of report). DIBC can be classified as

inherently biodegradable (Sponsor).

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
18.12.2003 (2)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	= 3.44 - measured/nominal
LC50	:	= 28.6 - measured/nominal
Limit test	:	
Analytical monitoring	:	no
Method	:	EPA OTS 797.1400
Year	:	2002
GLP	:	yes
Test substance	:	other TS

Method : This study evaluated the acute toxicity of the test substance to rainbow trout (Onchorynchus mykiss Walbaum) over a 96-hour exposure period under static conditions. A preliminary study found 100% mortality at nominal concentrations of 50 and 100 mg DIBC/L and no deaths at 2.5 or 25 mg/L after 96 hr. Based on this preliminary study, the test solutions for the definitive study were prepared in duplicate at nominal concentrations of 3.44, 6.19, 11.1, 20.1, 36.1 and 65.0 mg/l. All concentrations were prepared without correction for purity. Duplicate negative control solutions (dilution water) were maintained concurrently. Dilution water was Lake Huron water supplied to the laboratory by the City of Midland Water Treatment Plant, subsequently sand-filtered, pH-adjusted with gaseous CO2, carbon-filtered and UV-irradiated, and monitored regularly. The dilution water used in this study was characterized as follows: TOC < 1000 mg/L, hardness of 72 mg/l as CaCO3, alkalinity of ~42 mg/l as CaCO3, pH of 7.3, conductivity of 190 mmhos/cm and chlorine <1 mg/l. Test vessels were 12-l glass beakers which were filled with 10 l of test solution. Ten fish were impartially introduced to each replicate test vessel at test initiation. Loading did not exceed 0.5-g fish per liter of test solution. Fish were not fed during the study. Terminal body weight and standard length were recorded for all surviving fish at test termination. Fish were observed daily for mortality and sublethal effects. Mortality was defined as a lack of response to prodding of the caudal peduncle accompanied by an absence of opercular movement. Dissolved oxygen, pH and temperature were recorded at test initiation and daily thereafter.

The U.S. EPA Trimmed Spearman-Karber Program, v. 1.5, using nominal DIBC concentrations was used to calculate the LC50 values and corresponding percent trim values. The NOEC was determined as the highest exposure concentration that exhibited 0% mortality or sublethal effects.

Remark : Mortality in the 65, 36.1 and 6.19 mg/l treatment groups was 100, 85 and 5% after 72 and 96 hours of exposure. No deaths occurred at 11.1 or 20.1 mg/L. Sublethal effects at 6.19 to 36.1 mg/L included partial to complete loss of equilibrium, lethargy and immobility. The temperature, pH and dissolved oxygen concentration during this study were maintained at 12.3 ± 0.2°C, 7.0 ± 0.3 and 9.2 ± 0.6 mg/l (or >72% saturation), respectively. Pooled standard length and weight means (± sd) for all surviving fish (treatments and controls) were 35 ± 2 mm and 518 ± 110 mg, respectively.

Result : LC50 (24-hr) = 31.2 mg/l (95% confidence interval = 27.8 - 35.0 mg/l);
LC50 (48-hr) = 29.4 mg/l (95% confidence interval = 26.8 - 32.3 mg/l);
LC50 (72-hr) = 28.6 mg/l (95% confidence interval = 25.6 - 31.9 mg/l);
LC50 (96-hr) = 28.6 mg/l (95% confidence interval = 25.6 - 31.9 mg/l)
The Spearman-Karber Trim was 0% for LC50 at 24, 48, 72 and 96 hours.

Test substance : See Section 1.1

DIBC + DMH = 99.4%

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
07.12.2003 (4)

Type :
Species :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 10.326 - calculated
Method : other: EPIWIN (v 3.10) ECOSAR Submodel (v 0.99g)
Year : 2003
GLP :
Test substance :

Remark : The EPIWIN model was run using the following measured physical chemical properties:
Vapor pressure (mm Hg) = 0.19515;
Boiling point (deg C) = 177.85; and
Melting point (deg C) = -65.15.
21.11.2003 (9)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : 17.5 - measured/nominal
EC50 : 47.8 - measured/nominal
Analytical monitoring : no
Method : EPA OTS 797.1300
Year : 2002
GLP : yes
Test substance : other TS

Method : This study evaluated the acute toxicity of the test substance to <24-hour old daphnia (Daphnia magna Straus) over a 48-hour exposure period under static conditions. A preliminary study found 90 or 100% immobility/mortality at nominal concentrations of 50, 100, 500 and 1000 mg DIBC/L and no effects at 1.0, 2.5, 10, or 25 mg/L after 48 hr. Based on this preliminary study, the test solutions for the definitive study were prepared in duplicate at nominal concentrations of 4.38, 8.75, 17.5, 35.0, 70.0 and 140 mg/l. All concentrations were prepared without correction for purity. Duplicate negative control solutions (dilution water) were maintained concurrently. Dilution water was Lake Huron water supplied to the laboratory by the City of Midland Water Treatment Plant, subsequently sand-filtered, pH-adjusted with gaseous CO2, carbon-filtered and UV-irradiated, adjusted to hardness of 172 mg/l as CaCO3, then autoclaved at 250°F and 18 psi for 30 min. The dilution water used in this study was characterized as follows: TOC < 1000 ug/L, hardness of 172 mg/l as CaCO3, alkalinity of ~38 mg/l as CaCO3, pH of 7.4, conductivity of 390 mmhos/cm and chlorine <1 ug/l. Test vessels were 250-ml glass jars containing 250 ml of test solution. Ten daphnia were impartially introduced to each replicate test vessel at test initiation. Terminal body weight and standard length were recorded for all surviving fish at test termination. Daphnia were observed every 24 hours for immobility, mortality and any other sublethal effects. Immobility was defined as the inability to swim within 15 seconds after gentle agitation of the test container. Dissolved oxygen, pH and temperature were recorded every 24 hours.

The U.S. EPA Probit Program, v. 1.5, using nominal DIBC concentrations, was used to calculate the EC50 values and corresponding slope values. If the Probit Program could not be used, the U.S. EPA Trimmed Spearman-Karber Program, v. 1.5, using nominal DIBC concentrations was used to calculate the EC50 values and corresponding percent trim values. The NOEC was determined as the highest exposure concentration that exhibited 0% mortality or sublethal effects.

Remark	:	Mortalities in the 140, 70.0 and 35.0 mg/l treatment groups were 100, 85 and 10% after 48 hours of exposure. The death in the 4.35 mg/l treatment group was believed to be accidental, attributed to the organism getting stuck to the vessel side, and was therefore excluded from the statistical evaluation. Immobilization was only reported for 2 daphnia in the 35.0 mg/l treatment group. The light intensity, temperature, pH and dissolved oxygen concentration during this study were maintained at 1784 ± 21 lux, 20.4 ± 0.2°C, 7.5 ± 0.1 and 8.7 ± 0.1 mg/l (or >97% saturation), respectively.
Result	:	EC50 (24-hr) = 86.2 mg/l (95% confidence interval = 76.1 - 97.6 mg/l; Spearman-Karber Trim = 0%); EC50 (48-hr) = 47.8 mg/l (95% confidence interval = 40.1 - 57.1 mg/l; Probit slope = 6.5 ± 2.6%)
Test substance	:	See Section 1.1 DIBC + DMH = 99.4%
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

07.12.2003 (3)

Type	:	
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 11.922 - calculated
Method	:	other: EPIWIN (v 3.10) ECOSAR Submodel (v 0.99g)
Year	:	2003
GLP	:	
Test substance	:	

Remark	:	The EPIWIN model was run using the following measured physical chemical properties: Vapor pressure (mm Hg) = 0.19515; Boiling point (deg C) = 177.85; and Melting point (deg C) = -65.15.

21.11.2003 (9)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other
Exposure period	:	96 hour(s)
Unit	:	mg/l
Limit test	:	
Analytical monitoring	:	no
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	2002
GLP	:	yes
Test substance	:	other TS

Method	:	This study evaluated effects of the test substance on algal growth over a 96-hour exposure period under static conditions. In two range-finding tests of concentrations ranging from 9.38 to 600 mg/L (Test 1) and 0.06 to 600 mg/L (Test 2) the 50% inhibitory effect level was between 9.38 and 18.75

mg/L at 72 and 96 hours. The test solutions were prepared at nominal concentrations of 0.25, 0.61, 1.54, 3.84, 9.6, 24 and 60 mg/l in filter-sterilized algal growth medium. Negative control solutions (medium only) were also maintained concurrently. Test vessels were 250-ml Erlenmeyer flasks plugged w/ foam and contained 50 ml of test solution. Each of four replicated per treatment and control were inoculated with 3-7 day old algal culture to achieve 1x104 cells/ml. Treatment and control solutions were incubated in a growth chamber at 24 ± 2°C under continuous illumination at 8 ± 20% kLux. Temperature and pH were recorded at test initiation and termination. Cell numbers were measured daily using a haemocytometer. Biomass (as area under the growth curve) and growth rate were calculated from cell counts.

Nominal concentrations of DIBC were used for all calculations. The EC50 values were determined using the TOXSTAT program.

Result :

Endpoint	Hours	EC50 (95% Conf. Interval)	NOEC (mg/l)	LOEC (mg/l)
Cell Numbers	72	6.97 (5.68, 7.90)	1.54	3.84
Cell Numbers	96	9.41(7.17, 11.87)	3.84	9.6
Biomass *	72	6.62 (5.85, 7.44)	0.25	0.61
Biomass *	96	7.41 (6.55, 8.22)	1.54	3.84
Growth Rate	0-72	19.62 (15.14, 25.43)	3.84	9.6
Growth Rate	0-96	29.95 (25.46, 33.75)	3.84	9.6

* Biomass = area under the growth curve.

Test substance : Purity: DIBC + DMH = 98.34 ± 0.03%
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
07.12.2003 (6)

Species : other algae: green algae
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = 7.931 - calculated
Method : other: EPIWIN (v 3.10) ECOSAR Submodel (v 0.99g)
Year : 2003
GLP :
Test substance :

Remark : The EPIWIN model was run using the following measured physical chemical properties:
Vapor pressure (mm Hg) = 0.19515;
Boiling point (deg C) = 177.85; and
Melting point (deg C) = -65.15.
21.11.2003 (9)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 3560 - mg/kg bw
Species	:	rat
Strain	:	no data
Sex	:	male
Number of animals	:	20
Vehicle	:	other: Tergitol 7
Doses	:	1000, 2000, 3980 and 7950 mg/kg body weight
Method	:	other: see remark
Year	:	1948
GLP	:	no
Test substance	:	other TS
Remark	:	A 20% dispersion of the test substance in 1.0% Tergitol 7 was administered by stomach tube to 5 male albino rats per group. Dose concentrations were 1000, 2000, 3980 and 7950 mg/kg body weight. Animals were observed for mortality for 14 days following dosing. Body weights were obtained on the day of dosing and on day 14.
Result	:	LD50 = 3560 mg/kg body weight (95% confidence limit = 1430 to 8860 mg/kg body weight) The compound formed an unstable dispersion with "Tregitol" and the broad range for the LD50 may reflect, in part at least, inaccuracies in the individual doses. The number of deaths are indicated in the following table: Dose (mg/kg) Number dead/number dosed 1000 0/5 2000 2/5 3980 3/5 7950 3/5 All deaths occurred within one to eight days following dosing. Death followed each instance when prostration or narcosis occurred following dosing. All surviving animals gained weight over the 14 days following dosing.
Test substance	:	diisobutyl carbinol - additional information not provided
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

09.12.2003 (1)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	other
Value	:	-
Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	12
Vehicle	:	
Doses	:	saturated vapor or cooled mist (approximately 400 ppm)
Exposure time	:	8 hour(s)
Method	:	other: see remark

Year	:	1948
GLP	:	no
Test substance	:	other TS
Remark	:	Two separate 8-hour inhalation exposure studies were conducted with six rats in each study. In one study, the animals were exposed to a saturated vapor, produced at room temperature. In another study, the test atmosphere was a cooled mist, produced by heating the test substance to 170 degrees C while air was bubbled through it.
Result	:	All 12 rats survived the exposures.
Test condition	:	diisobutyl carbinol - additional information not provided

09.12.2003 (1)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	= 4591 - mg/kg bw
Species	:	rabbit
Strain	:	no data
Sex	:	male
Number of animals	:	20
Vehicle	:	other: none
Doses	:	2.52, 5, 10 and 20 ml/kg body weight
Method	:	other: see remark
Year	:	1948
GLP	:	no
Test substance	:	other TS
Remark	:	The undiluted test substance was applied as a single dose to 4 groups of 10 male albino rabbits each at the following dose levels: 2.52, 5.0, 10 and 20 ml/kg, which correlates to doses of 2044, 4056, 8112 and 16,224 mg/kg, respectively (density = 0.8112 g/cm3). The test material was applied, undiluted at the appropriate dose, under an impervious sheeting. The animals remained exposed to the test substance for 24 hours. Rabbits were observed for 14 days and body weights were obtained on the day of application and on day 14.
Result	:	LD50 = 4591 mg/kg body weight (95% confidence limits = 2036 to 10383 mg/kg body weight). The number of deaths are indicated in the following table: Dose (ml/kg) Number dead/number dosed 2.52 1/5 5 2/5 10 4/5 20 4/5 All deaths occurred between 2 and 11 days following application. Marked erythema and in some instances, necrosis of the skin were noted. Livers showed varying degrees of congestion and the kidneys were usually pale. All surviving rabbits lost weight over the 14 day post-exposure period.
Test substance	:	diisobutyl carbinol - additional information not provided
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

09.12.2003 (1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA98, TA100, TA1538, TA1537; Escherichia coli tester strain WP2uvrA.
Test concentration	:	3.33, 10.0, 33.3, 100, 333 and 1000 ug/plate (with S9 mix); 1.00, 3.33, 10.0, 33.3, 100 and 500 ug/plate (without S9 mix)
Cycotoxic concentr.	:	>= 333 ug/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: EEC Directive 2000/32/EC; OECD Method 471; U.S. EPA OPPTS Method 870.5100.
Year	:	2002
GLP	:	yes
Test substance	:	other TS
Method	:	The preincubation assay was conducted with six concentrations of DIBC in both the presence and absence of microsomal enzymes prepared from Aroclor™-induced rat liver (S9 mix) along with concurrent vehicle and positive controls using three plates per concentration. A range finding study was conducted with strains TA-100 and WP2uvrA at 10 DIBC concentrations ranging from 6.67 to 5000 ug/plate with and without metabolic activation. Reduced or absent background lawn was observed at concentrations of 333 ug/plate and higher in both systems. The six concentrations tested in the mutagenicity assay with all tester strains ranged from 3.33 to 1000 ug per plate in the presence of S9 mix and from 1.00 to 500 ug per plate in the absence of S9 mix. Dimethylsulfoxide (DMSO) was the solvent for the test substance and served as the negative control. For the non-activation assay, the following positive control substances were used: Sodium azide (for strains TA1535 and TA100); 2-Nitrofluorene (for strain TA98); ICR-191 (for strain TA1537) and 4-nitroquinoline-N-oxide (for strain WP2uvrA). The positive control substance, 2-aminoanthracene was used for all tester strains with metabolic activation. The results of the initial mutagenicity assay were confirmed in an independent experiment. The criteria for evaluation were: at least a 2-fold (TA-100) or 3-fold (TA98, TA1535, TA1537, and WP2uvrA) concentration-related increase and reproducible increase in mean revertants per plate over the mean of the appropriate vehicle control was considered positive.
Result	:	No increase in revertants meeting the criteria for positive response was observed at any concentration in any strain with or without metabolic activation in either experiment. Under the conditions of this study, DIBC was not mutagenic to bacterial cells with or without metabolic activation.
Test substance	:	See Section 1.1: Purity: DIBC + DMH = 98.34%

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
07.12.2003 (5)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Carpenter, C.P. 1948. Range Finding Tests on Diisobutyl Carbinol. Unpublished Report Number 11-89. Mellon Institute of Industrial Research, University of Pittsburgh, PA, USA.

(2) Heim, D. 2003. Diisobutyl carbinol: Determination of Ready Biodegradability Using the Respirometry Method. Unpublished Report (ABC No. 47679; Dow No. 020112) for The Dow Chemical Company by ABC Laboratories, Inc., Columbia, MO, USA.

(3) Marino, T. A. and A. M. Yaroch. 2002. Diisobutyl Carbinol: An Acute Toxicity Study with the Daphnid, Daphnia magna Straus. Unpublished Report (Dow No. 021048) for Union Carbide Corporation by Toxicology & Environmental Research and Consulting, The Dow Chemical Company, Midland, MI, USA.

(4) Marino, T.A. and A. M. Yaroch. 2002. Diisobutyl Carbinol: An Acute Toxicity Study with the Rainbow Trout, Oncorhynchus mykiss Walbaum. Unpublished Report (Dow No. 021047) for Union Carbide Corporation by Toxicology & Environmental Research and Consulting, The Dow Chemical Company, Midland, MI, USA.

(5) Mecchi, M. S. 2002. Salmonella - Escherichia coli/Mammalian-Microsome Reverse Mutation Assay Preincubation Method with a Confirmatory Assay with Diisobutyl Carbinol. Unpublished Report (Covance Study No. 23500-0-422OECD; Dow No. 011222) for The Dow Chemical Company by Covance Laboratories Inc., Vienna, VA, USA.

(6) Roshon, R. 2002. Diisobutyl Carbinol: Growth Inhibition Test with the Freshwater Green Alga, Selenastrum capricornutum Printz. Unpublished Report (ESG Study No. S2287; Dow No. 020026) for the Dow Chemical Company by ESG International Inc., Guelph, Onterio, Canada.

(7) The Design Institute for Physical Properties (DIPPR) Information and Data Evaluation Manager, Version 1.5.0, Copyright BYU-TPL2000.

(8) U.S. Environmental Protection Agency. 2000. EPI Suite, Version 3.10; AOPWIN Program, Version 1.90; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

(9) U.S. Environmental Protection Agency. 2000. EPI Suite, Version 3.10; ECOSAR Version 0.99g; PC-Computer software developed by ECOSAR Program, Risk Assessment Division (7403), Washington, DC.

(10) U.S. Environmental Protection Agency. 2000. EPI Suite, Version 3.10; KOWWIN Program, Version 1.66; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

(11) U.S. Environmental Protection Agency. 2000. EPI Suite, Version 3.10; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

(12) Wilson, L.C. 2000. Liquid-Liquid Equilibrium Measurements for Eighteen Glycol Ethers, Ketones, Esters and Alcohols with Water. Project Report No. 44662, 10/13/2000. Union Carbide Corporation, S. Charleston, WV, USA.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT